Triisopropanolamine 122-20-3 | DTXSID5021415

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 5.88 days

Global applicability domain: Inside

Local applicability domain index: 5.24e-01

Confidence level: 7.81e-01

Nearest Neighbors from the Training Set

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Tetradeca-1,13-diene Measured: 367 Predicted: 8.69 Image not found

2,4-Dimethylheptane Measured: 61.9 Predicted: 4.29 Image not found

2-Methylheptane Measured: 12.5 Predicted: 3.99

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2-Methyloctane Measured: 40.7 Predicted: 4.23 Image not found

3-Methyloctane Measured: 40.7 Predicted: 4.08